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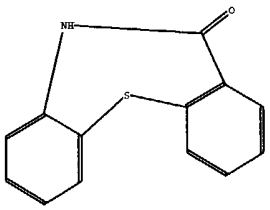

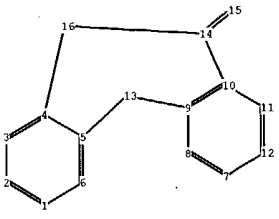

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ring nodes :
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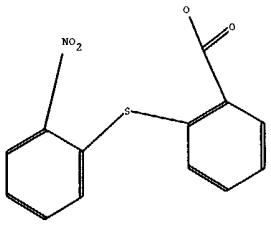
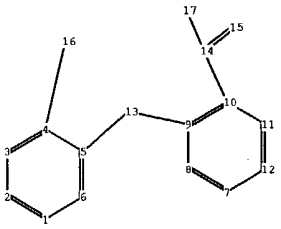
chain bonds :
14-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-16 5-6 5-13 7-8 7-12 8-9 9-10 9-13
10-11 10-14 11-12 14-16
exact/norm bonds :
4-16 5-13 9-13 10-14 14-15 14-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:Atom

C:\STNEXP4\QUERIES\10030251.str





chain nodes :
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ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
ring/chain nodes :
14
chain bonds :
4-16 5-13 9-13 14-15 14-17
ring/chain bonds :
10-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
5-13 9-13 10-14 14-15 14-17
exact bonds :
4-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:Atom
17:CLASS

```
=> d his

     (FILE 'HOME' ENTERED AT 14:35:10 ON 23 SEP 2003)

     FILE 'REGISTRY' ENTERED AT 14:35:16 ON 23 SEP 2003
L1                STRUCTURE UPLOADED
L2                QUE L1
L3              4 S L2
L4           1160 S 3068.74/RID
L5                SCREEN 2076
L6                STRUCTURE UPLOADED
L7                QUE L6 AND L5
L8              2 S L7
L9            112 S L2 SSS FUL
L10            37 S L7 SSS FUL

     FILE 'CAPLUS' ENTERED AT 14:45:23 ON 23 SEP 2003
L11            88 S L9
L12            44 S L10
L13            13 S L11 AND L12

     FILE 'REGISTRY' ENTERED AT 14:46:04 ON 23 SEP 2003

=> d l2
L2 HAS NO ANSWERS
L1                STR
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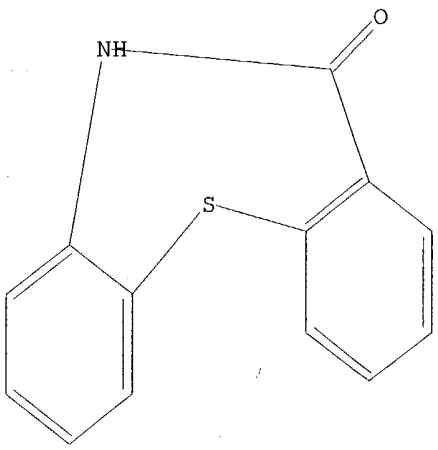


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Structure attributes must be viewed using STN Express query preparation.
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L7 HAS NO ANSWERS
L5                SCR 2076
L6                STR
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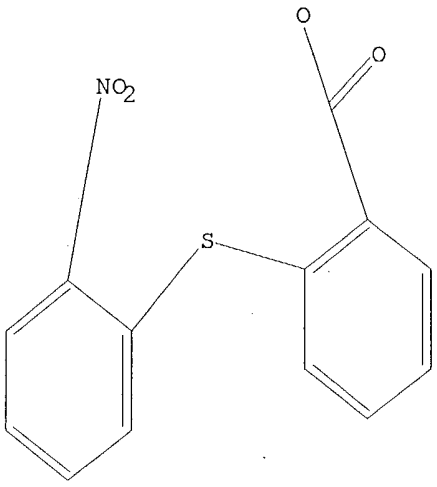

Structure attributes must be viewed using STN Express query preparation.
L7 QUE ABB=ON PLU=ON L6 AND L5

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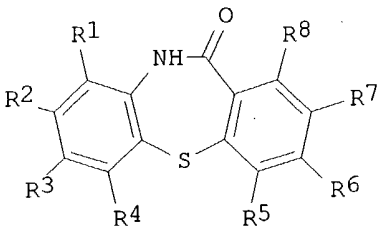
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

applicants

L13 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:463259 CAPLUS
DOCUMENT NUMBER: 131:102294
TITLE: Preparation of dibenzothiazepines and their intermediates
INVENTOR(S): Harada, Katsumasa; Nishino, Shigehide; Yoshii, Kiyotaka
PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11199574	A2	19990727	JP 1998-15022	19980109
WO 2001004106	A1	20010118	WO 1999-JP3719	19990709
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9946506	A1	20010130	AU 1999-46506	19990709
EP 1201663	A1	20020502	EP 1999-929773	19990709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
EE 200200014	A	20030415	EE 2002-14	19990709
NO 2002000059	A	20020304	NO 2002-59	20020107

PRIORITY APPLN. INFO.: JP 1998-15022 A 19980109
WO 1999-JP3719 A 19990709
OTHER SOURCE(S): CASREACT 131:102294; MARPAT 131:102294
GI



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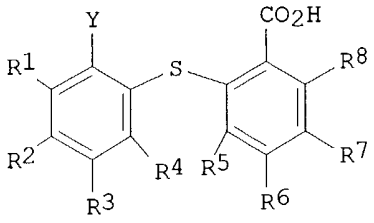
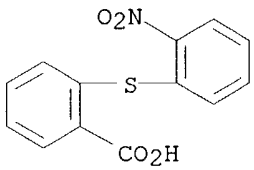


II

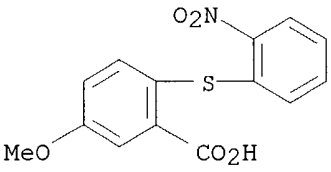
AB Dibenzothiazepines I [R1-R8 = H, (substituted) alkyl, alkoxy, alkylcarbonyl, aryl, aryloxy, arylcarbonyl], useful as intermediates for antipsychotic piperazinyldibenzothiazepine deriv., are prepd. by reaction of (substituted) 2-halonitrobenzenes with (substituted) thiosalicylic acids, redn. of the resulting II (R1-R8 = same as I; Y = NO2), and dehydrocondensation of II (Y = NH2). 2-Chloronitrobenzene was condensed with thiosalicylic acid in N,N-dimethylformamide using K2CO3 at 70.degree. for 6 h to give 98% II (R1-R8 = H, Y = NO2), which was reduced by H using Raney Ni and heated in refluxing PhMe to give I (R1-R8 = H).

IT **19806-43-0P 55114-91-5P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of dibenzothiazepines from halonitrobenzenes and thiosalicylic acids)

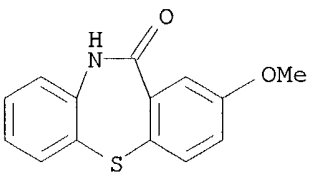
RN 19806-43-0 CAPLUS
CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



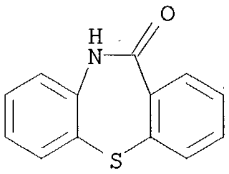
RN 55114-91-5 CAPLUS
CN Benzoic acid, 5-methoxy-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



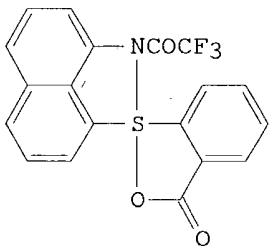
IT **3158-77-8P 3159-07-7P,** Dibenzo[b,f][1,4]thiazepin-11(10H)-one
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of dibenzothiazepines from halonitrobenzenes and thiosalicylic acids)
RN 3158-77-8 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methoxy- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 3159-07-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L13 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:435589 CAPLUS
DOCUMENT NUMBER: 121:35589
TITLE: Novel reactions of spirosulfurane precursor sulfides and sulfoxides
AUTHOR(S): Kuti, M.; Rabai, J.; Kapovits, I.
CORPORATE SOURCE: Dep. Org. Chem., L. Eotvos Univ., Budapest, H-1518, Hung.
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1993), 85(1-4), 119-27
CODEN: PSSLEC; ISSN: 1042-6507
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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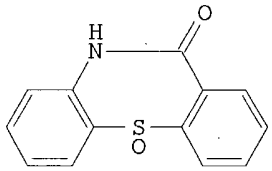

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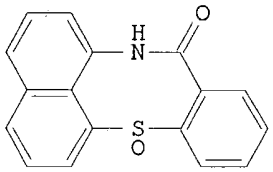

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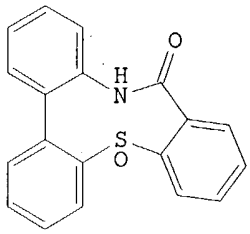
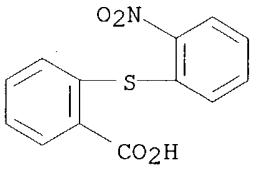


IV

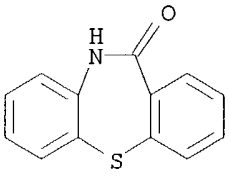
AB The SIv[C,C,N,O] spirosulfurane I and the lactam-sulfoxides II, III, and IV with seven-, eight- and nine-membered rings have been prepd. by oxidn. and dehydration of trifluoroacetylaminoarylcarboxyphenyl sulfides and sulfoxides, resp. A mechanism is proposed for the formation of lactam-sulfoxides. The prepn. of the starting sulfides and sulfoxides is also described.

IT **19806-43-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. by iron)

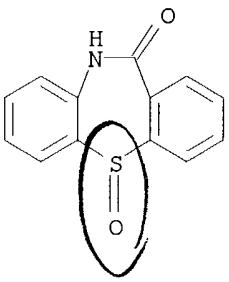
RN 19806-43-0 CAPLUS
CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



IT **3159-07-7P**, Dibenzo[b,f][1,4]thiazepin-11(10H)-one
20290-48-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 3159-07-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

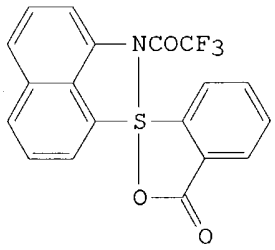


RN 20290-48-6 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5-oxide (8CI, 9CI) (CA INDEX NAME)



2813

L21 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:435589 CAPLUS
DOCUMENT NUMBER: **121:35589**
TITLE: Novel reactions of spirosulfurane precursor sulfides and sulfoxides
AUTHOR(S): Kuti, M.; Rabai, J.; Kapovits, I.
CORPORATE SOURCE: Dep. Org. Chem., L. Eotvos Univ., Budapest, H-1518, Hung.
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1993), 85(1-4), 119-27
CODEN: PSSLEC; ISSN: 1042-6507
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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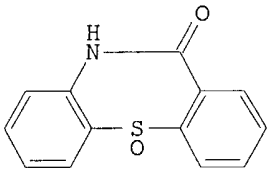

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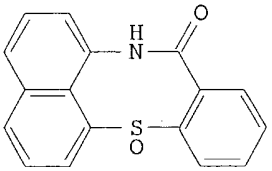
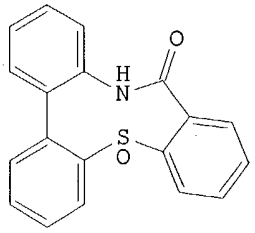


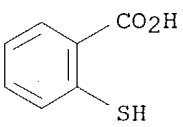
III



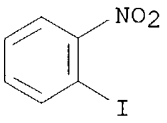
IV

AB The SIv[C,C,N,O] spirosulfurane I and the lactam-sulfoxides II, III, and IV with seven-, eight- and nine-membered rings have been prepared by oxidation and dehydration of trifluoroacetylaminoarylcarboxyphenyl sulfides and sulfoxides, resp. A mechanism is proposed for the formation of lactam-sulfoxides. The preparation of the starting sulfides and sulfoxides is also described.

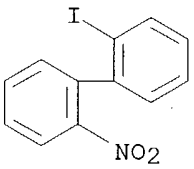
IT **147-93-3**, Thiosalicylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with iodonitrobenzene, iodonitrobiphenyl, and bromonaphthyltrifluoroacetamide)
RN 147-93-3 CAPLUS
CN Benzoic acid, 2-mercapto- (9CI) (CA INDEX NAME)



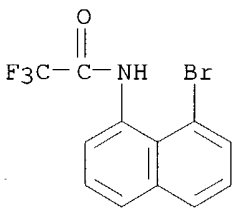
IT **609-73-4**, 1-Iodo-2-nitrobenzene **35882-95-2**,
1,1'-Biphenyl, 2-iodo-2'-nitro- **155882-83-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with thiosalicylic acid)
RN 609-73-4 CAPLUS
CN Benzene, 1-iodo-2-nitro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



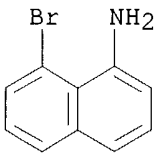
RN 35882-95-2 CAPLUS
CN 1,1'-Biphenyl, 2-iodo-2'-nitro- (9CI) (CA INDEX NAME)



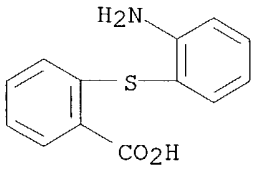
RN 155882-83-0 CAPLUS
CN Acetamide, N-(8-bromo-1-naphthalenyl)-2,2,2-trifluoro- (9CI) (CA INDEX NAME)



IT **62456-34-2P**, 1-Naphthalenamine, 8-bromo- **114724-41-3P**
155586-27-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and acylation by trifluoroacetic anhydride)
RN 62456-34-2 CAPLUS
CN 1-Naphthalenamine, 8-bromo- (9CI) (CA INDEX NAME)

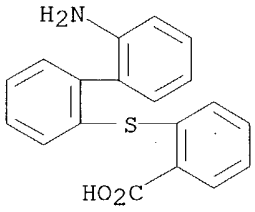


RN 114724-41-3 CAPLUS
CN Benzoic acid, 2-[(2-aminophenyl)thio]-, hydrochloride (9CI) (CA INDEX NAME)



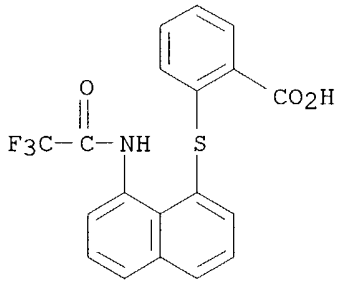
● HCl

RN 155586-27-9 CAPLUS
CN Benzoic acid, 2-[(2'-amino[1,1'-biphenyl]-2-yl)thio]-, hydrochloride (9CI) (CA INDEX NAME)

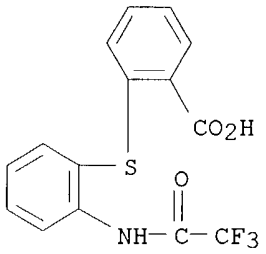


● HCl

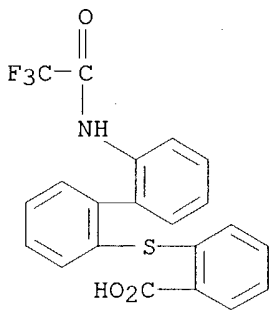
IT **155882-75-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and oxidation by phenyltrimethylammonium bromide)
RN 155882-75-0 CAPLUS
CN Benzoic acid, 2-[[8-[(trifluoroacetyl)amino]-1-naphthalenyl]thio]- (9CI) (CA INDEX NAME)



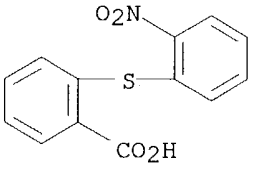
IT **155882-74-9P 155882-76-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and oxidation by tert-Bu hypochlorite)
RN 155882-74-9 CAPLUS
CN Benzoic acid, 2-[[2-[(trifluoroacetyl)amino]phenyl]thio]- (9CI) (CA INDEX NAME)



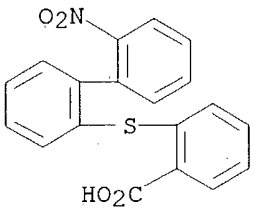
RN 155882-76-1 CAPLUS
CN Benzoic acid, 2-[[2'-[(trifluoroacetyl)amino][1,1'-biphenyl]-2-yl]thio]- (9CI) (CA INDEX NAME)



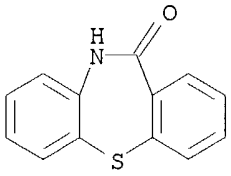
IT **19806-43-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reduction by iron)
RN 19806-43-0 CAPLUS
CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



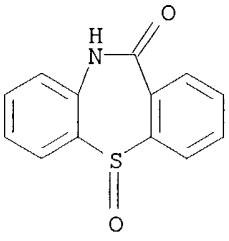
IT **155882-80-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reduction with iron)
RN 155882-80-7 CAPLUS
CN Benzoic acid, 2-[(2'-nitro[1,1'-biphenyl]-2-yl)thio]- (9CI) (CA INDEX NAME)



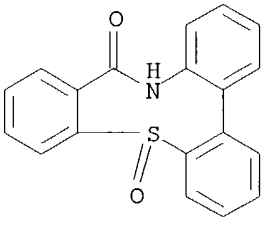
IT **3159-07-7P**, Dibenzo[b,f][1,4]thiazepin-11(10H)-one
20290-48-6P 155586-25-7P 155882-81-8P
155882-82-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 3159-07-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



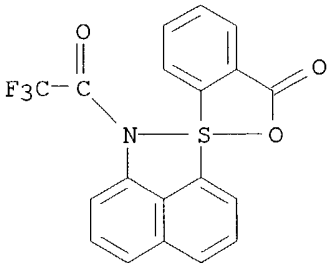
RN 20290-48-6 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5-oxide (8CI, 9CI) (CA INDEX NAME)



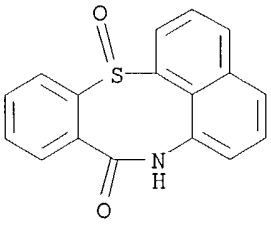
RN 155586-25-7 CAPLUS
CN Tribenzo[b,f,h][1,5]thiazonin-10(11H)-one, 5-oxide (9CI) (CA INDEX NAME)



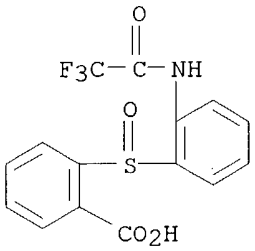
RN 155882-81-8 CAPLUS
CN Spiro[3H-2,1-benzoxathiole-1,1'λ4-[2H]naphth[1,8-cd]isothiazol]-3-one, 2'-(trifluoroacetyl)- (9CI) (CA INDEX NAME)



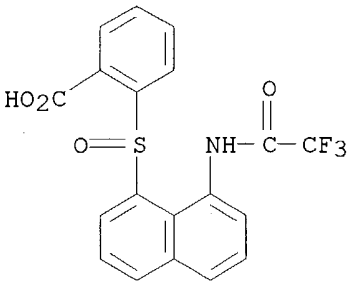
RN 155882-82-9 CAPLUS
CN Benzo[g]naphtho[1,8-bc][1,5]thiazocin-8(7H)-one, 13-oxide (9CI) (CA INDEX NAME)



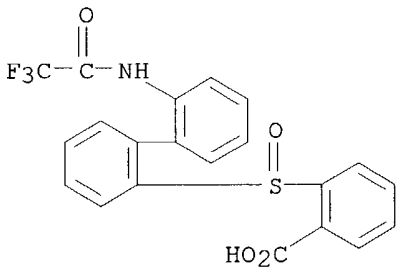
IT **155882-77-2P 155882-78-3P 155882-79-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as spirosulfurane precursor)
RN 155882-77-2 CAPLUS
CN Benzoic acid, 2-[[2-[(trifluoroacetyl)amino]phenyl]sulfinyl]- (9CI) (CA INDEX NAME)



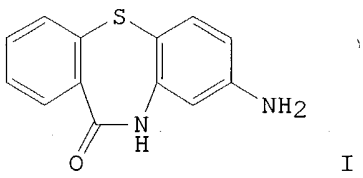
RN 155882-78-3 CAPLUS
CN Benzoic acid, 2-[[8-[(trifluoroacetyl)amino]-1-naphthalenyl]sulfinyl]- (9CI) (CA INDEX NAME)



RN 155882-79-4 CAPLUS
CN Benzoic acid, 2-[[2'-[(trifluoroacetyl)amino][1,1'-biphenyl]-2-yl]sulfinyl]- (9CI) (CA INDEX NAME)



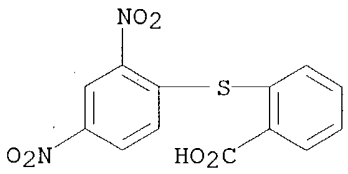
L13 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1986:626505 CAPLUS
DOCUMENT NUMBER: 105:226505
TITLE: Synthesis and structural studies of 8-amino-10,11-dihydro-5H-dibenzo[b,e][1,4]thiazepine-11-one
AUTHOR(S): Joshi, B. C.; Pande, Jyoti
CORPORATE SOURCE: Chem. Lab., Univ. Rajasthan, Jaipur, 302004, India
SOURCE: Chemistry & Industry (London, United Kingdom) (1985), (24), 825-6
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:226505
GI



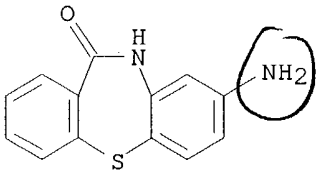
I

AB o-HO2CC6H4SC6H3(O2N)2-2,4, prepd. from o-HSC6H4CO2H and 2,4-(O2N)2C6H3Cl was reduced to o-HO2CC6H4SC6H3(NH2)2-2,4, which was cyclized by H3PO4 to give the title compd.(I).

IT **33840-90-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
RN 33840-90-3 CAPLUS
CN Benzoic acid, 2-[(2,4-dinitrophenyl)thio]- (9CI) (CA INDEX NAME)

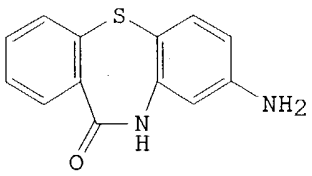


IT **105554-89-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectra of)
RN 105554-89-0 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-amino- (9CI) (CA INDEX NAME)


O
H
N
NH2
S

3913

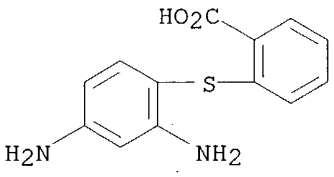
L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1986:626505 CAPLUS
DOCUMENT NUMBER: **105:226505**
TITLE: Synthesis and structural studies of 8-amino-10,11-dihydro-5H-dibenzo[b,e][1,4]thiazepine-11-one
AUTHOR(S): Joshi, B. C.; Pande, Jyoti
CORPORATE SOURCE: Chem. Lab., Univ. Rajasthan, Jaipur, 302004, India
SOURCE: Chemistry & Industry (London, United Kingdom) (1985), (24), 825-6
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:226505
GI



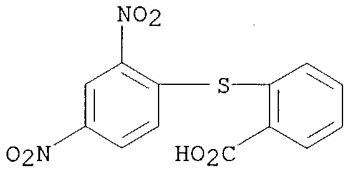
I

AB o-HO2CC6H4SC6H3(O2N)2-2,4, prepared from o-HSC6H4CO2H and 2,4-(O2N)2C6H3Cl was reduced to o-HO2CC6H4SC6H3(NH2)2-2,4, which was cyclized by H3PO4 to give the title compound(I).

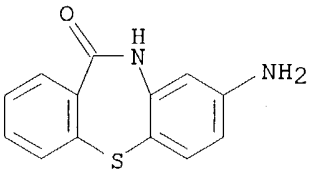
IT **105554-88-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. cyclization of, dibenzothiazepinone derivative from)
RN 105554-88-9 CAPLUS
CN Benzoic acid, 2-[(2,4-diaminophenyl)thio]- (9CI) (CA INDEX NAME)



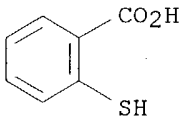
IT **33840-90-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 33840-90-3 CAPLUS
CN Benzoic acid, 2-[(2,4-dinitrophenyl)thio]- (9CI) (CA INDEX NAME)



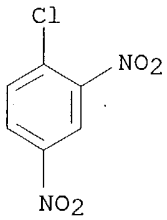
IT **105554-89-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectra of)
RN 105554-89-0 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-amino- (9CI) (CA INDEX NAME)



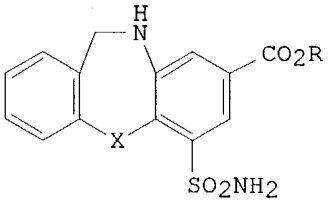
IT **147-93-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorodinitrobenzene)
RN 147-93-3 CAPLUS
CN Benzoic acid, 2-mercapto- (9CI) (CA INDEX NAME)



IT **97-00-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with mercaptoacetic acid)
RN 97-00-7 CAPLUS
CN Benzene, 1-chloro-2,4-dinitro- (8CI, 9CI) (CA INDEX NAME)



L13 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:499969 CAPLUS
DOCUMENT NUMBER: 89:99969
TITLE: 8-Carboxy-6-sulfamyldibenz[b,f][1,4]oxazepines and -thiazepines as potential high-ceiling diuretics
AUTHOR(S): Allen, Richard C.; Reitano, Philip A.; Urbach, Hansjoerg
CORPORATE SOURCE: Chem. Res. Dep., Hoechst-Roussel Pharm. Inc., Somerville, NJ, USA
SOURCE: Journal of Medicinal Chemistry (1978), 21(8), 838-40
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

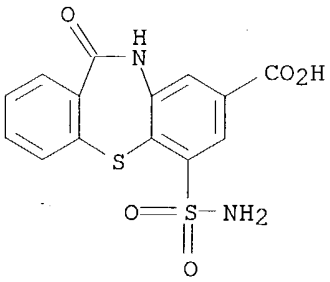


I

AB Five title compds. I (X = O or S, Y = O or H2, R = H or Me), conformationally rigid analogs of furosemide [54-31-9], were synthesized and tested for diuretic activity. Only I; (X = Y = O, R = Me) [66984-09-6] and I; (X = O, Y = H2, R = H) [66984-10-9] had natriuretic activity in rats and none of the compds. increased urinary vol. Apparently, conformational mobility of the 4-substituent of 3-amino-5-sulfamylbenzoates is required for diuretic activity.

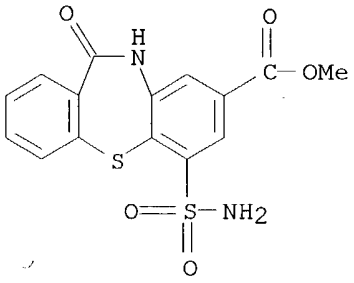
IT **66983-99-1P 66984-00-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and diuretic activity of)

RN 66983-99-1 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-11-oxo- (9CI) (CA INDEX NAME)

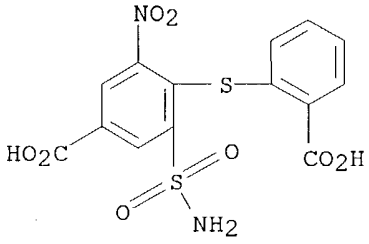


RN 66984-00-7 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-11-oxo-, methyl ester (9CI) (CA INDEX NAME)

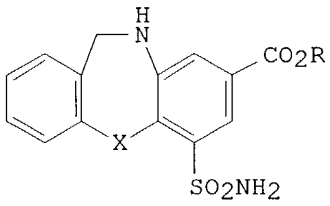


IT **66983-97-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
RN 66983-97-9 CAPLUS
CN Benzoic acid, 3-(aminosulfonyl)-4-[(2-carboxyphenyl)thio]-5-nitro- (9CI) (CA INDEX NAME)



4913

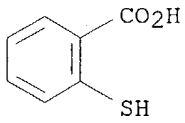
L15 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:499969 CAPLUS
DOCUMENT NUMBER: **89:99969**
TITLE: 8-Carboxy-6-sulfamyldibenz[b,f][1,4]oxazepines and -thiazepines as potential high-ceiling diuretics
AUTHOR(S): Allen, Richard C.; Reitano, Philip A.; Urbach, Hansjoerg
CORPORATE SOURCE: Chem. Res. Dep., Hoechst-Roussel Pharm. Inc., Somerville, NJ, USA
SOURCE: Journal of Medicinal Chemistry (1978), 21(8), 838-40
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 89:99969
GI



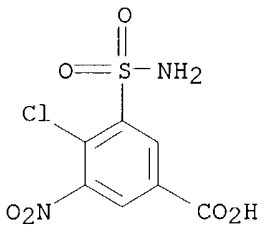
I

AB Five title compds. I (X = O or S, Y = O or H2, R = H or Me), conformationally rigid analogs of furosemide [**54-31-9**], were synthesized and tested for diuretic activity. Only I; (X = Y = O, R = Me) [**66984-09-6**] and I; (X = O, Y = H2, R = H) [**66984-10-9**] had natriuretic activity in rats and none of the compds. increased urinary volume Apparently, conformational mobility of the 4-substituent of 3-amino-5-sulfamylbenzoates is required for diuretic activity.

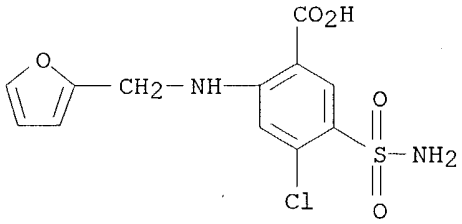
IT **147-93-3**
RL: BIOL (Biological study)
(condensation of, with chloronitrosulfamylbenzoate)
RN 147-93-3 CAPLUS
CN Benzoic acid, 2-mercapto- (9CI) (CA INDEX NAME)



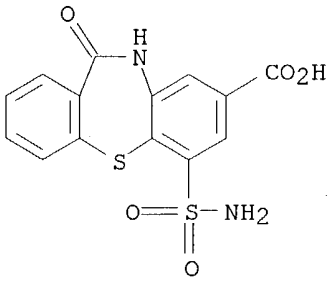
IT **22892-96-2**
RL: BIOL (Biological study)
(condensation of, with thiosalicylate)
RN 22892-96-2 CAPLUS
CN Benzoic acid, 3-(aminosulfonyl)-4-chloro-5-nitro- (9CI) (CA INDEX NAME)



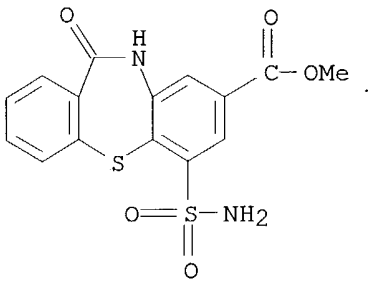
IT **54-31-9DP**, analog **66983-99-1P 66984-00-7P 66984-01-8P 66984-07-4DP**, derivs. **66984-08-5DP**, derivs. **66984-09-6P 66984-10-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and diuretic activity of)
RN 54-31-9 CAPLUS
CN Benzoic acid, 5-(aminosulfonyl)-4-chloro-2-[(2-furanylmethyl)amino]- (9CI) (CA INDEX NAME)



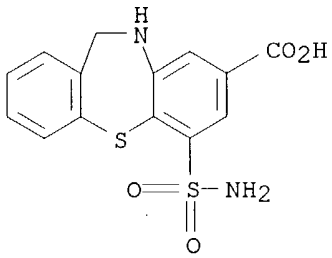
RN 66983-99-1 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-11-oxo- (9CI) (CA INDEX NAME)



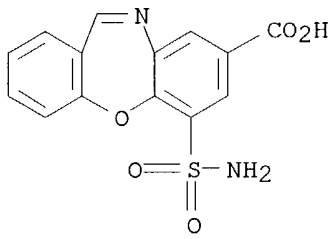
RN 66984-00-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-11-oxo-, methyl ester (9CI) (CA INDEX NAME)



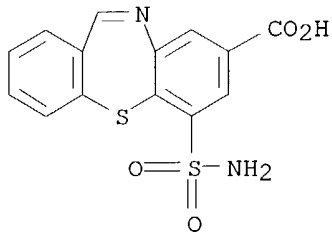
RN 66984-01-8 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro- (9CI) (CA INDEX NAME)



RN 66984-07-4 CAPLUS
CN Dibenz[b,f][1,4]oxazepine-8-carboxylic acid, 6-(aminosulfonyl)- (9CI) (CA INDEX NAME)

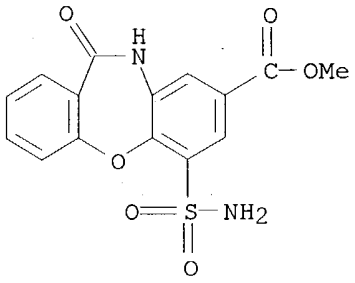


RN 66984-08-5 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)- (9CI) (CA INDEX NAME)

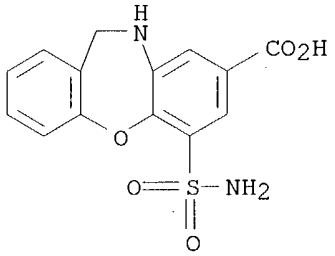


RN 66984-09-6 CAPLUS

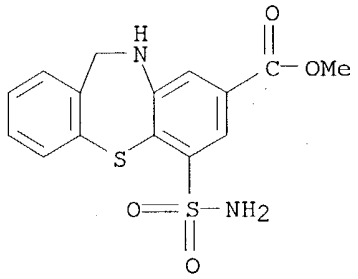
CN Dibenz[b,f][1,4]oxazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-11-oxo-, methyl ester (9CI) (CA INDEX NAME)



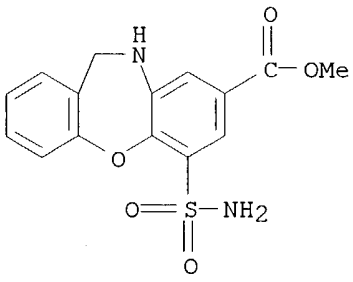
RN 66984-10-9 CAPLUS
CN Dibenz[b,f][1,4]oxazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro- (9CI) (CA INDEX NAME)



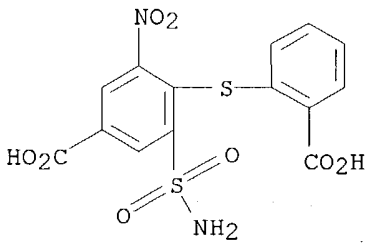
IT **66984-03-0P 66984-05-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 66984-03-0 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-, methyl ester (9CI) (CA INDEX NAME)



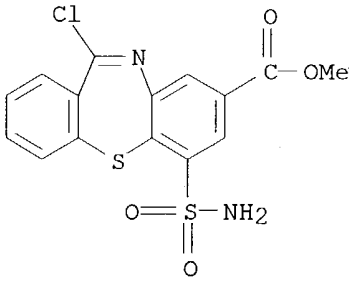
RN 66984-05-2 CAPLUS
CN Dibenz[b,f][1,4]oxazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-, methyl ester (9CI) (CA INDEX NAME)



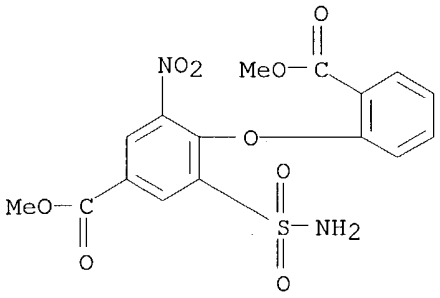
IT **66983-97-9P 66984-02-9P 66984-04-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 66983-97-9 CAPLUS
CN Benzoic acid, 3-(aminosulfonyl)-4-[(2-carboxyphenyl)thio]-5-nitro- (9CI) (CA INDEX NAME)



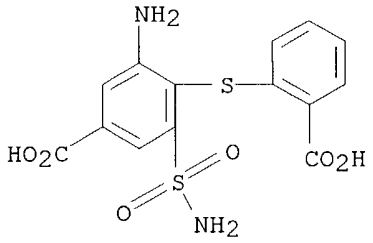
RN 66984-02-9 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-11-chloro-, methyl ester (9CI) (CA INDEX NAME)



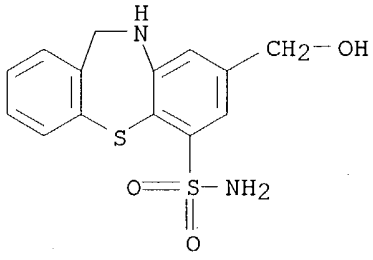
RN 66984-04-1 CAPLUS
CN Benzoic acid, 3-(aminosulfonyl)-4-[2-(methoxycarbonyl)phenoxy]-5-nitro-, methyl ester (9CI) (CA INDEX NAME)



IT **66983-98-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal cyclodehydration of)
RN 66983-98-0 CAPLUS
CN Benzoic acid, 3-amino-5-(aminosulfonyl)-4-[(2-carboxyphenyl)thio]- (9CI) (CA INDEX NAME)



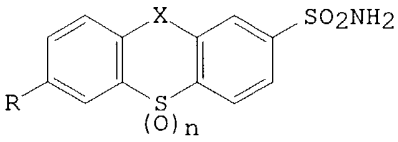
IT **66984-06-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 66984-06-3 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-6-sulfonamide, 10,11-dihydro-8-(hydroxymethyl)- (9CI) (CA INDEX NAME)



L13 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:22940 CAPLUS
DOCUMENT NUMBER: 88:22940
TITLE: Tricyclic sulfonamides
INVENTOR(S): Cross, Peter Edward; Dickinson, Roger Peter
PATENT ASSIGNEE(S): Pfizer Ltd., UK
SOURCE: Brit., 13 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1480553	A	19770720	GB 1975-25129	19760603

PRIORITY APPLN. INFO.: GB 1975-25129 19760603
GI

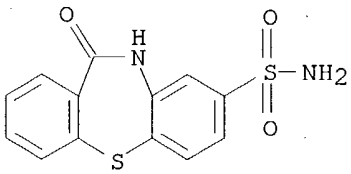


I

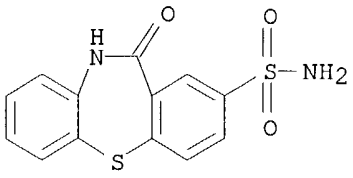
AB Seventeen title compds. I (R = H, Cl, CF3; X = bond, CH2, NAc, NH, CONH, NHCO, CO, NH; n = 0, 2), useful as cerebral vasodilators (no data), were prepd. by std. methods. E.g., thioxanthene-2-sulfonyl chloride with excess NH3 gave I (R = H, X = CH2, n = 0) which on H2O2 oxidn. in AcOH gave I (R = H, X = CH2, n = 2). I (R = Cl, X = NAc, n = 0) was prepd. from [2,4-(H2N)(H2NSO2)C6H3]2S by sequential treatment with 2,5-Cl2C6H3NO2, acetylation, and refluxing with alc. KOH in Me2CO. Many I show anticonvulsant activity (no data).

IT **65192-76-9P 65192-80-5P 65192-85-0P**
65192-86-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(cerebral vasodilator, prepn. of)

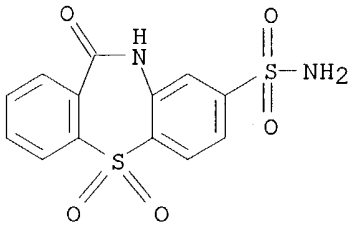
RN 65192-76-9 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-8-sulfonamide, 10,11-dihydro-11-oxo- (9CI) (CA INDEX NAME)



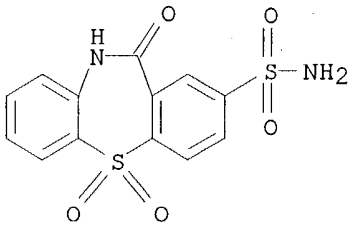
RN 65192-80-5 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-2-sulfonamide, 10,11-dihydro-11-oxo- (9CI) (CA INDEX NAME)



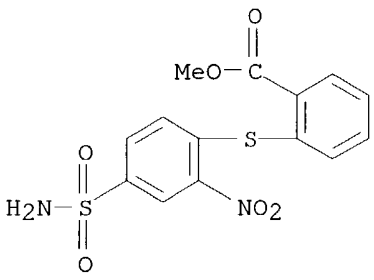
RN 65192-85-0 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-8-sulfonamide, 10,11-dihydro-11-oxo-, 5,5-dioxide (9CI) (CA INDEX NAME)



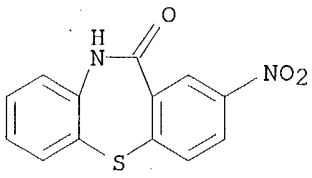
RN 65192-86-1 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine-2-sulfonamide, 10,11-dihydro-11-oxo-, 5,5-dioxide (9CI) (CA INDEX NAME)



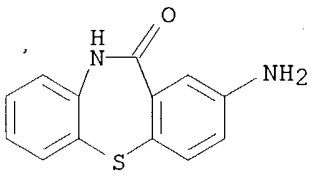
IT **65192-74-7P 65192-78-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
RN 65192-74-7 CAPLUS
CN Benzoic acid, 2-[[4-(aminosulfonyl)-2-nitrophenyl]thio]-, methyl ester (9CI) (CA INDEX NAME)



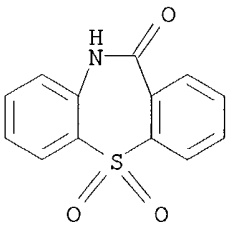
RN 65192-78-1 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-nitro- (9CI) (CA INDEX NAME)



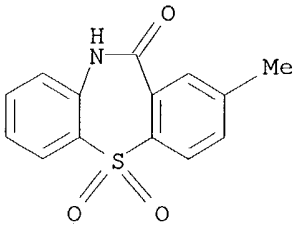
IT **65192-79-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and sulfamoylation of)
RN 65192-79-2 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-amino- (9CI) (CA INDEX NAME)



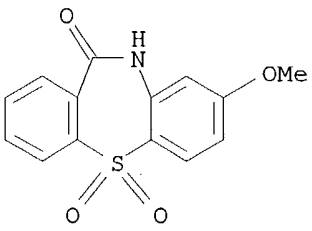
L13 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1976:105557 CAPLUS
DOCUMENT NUMBER: 84:105557
TITLE: A novel synthesis of dibenzo[b,f][1,4]thiazepin-11(10H)one 5,5-dioxides
AUTHOR(S): Bennett, O. Francis; Johnson, James; Galletto, Sandra
CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, USA
SOURCE: Journal of Heterocyclic Chemistry (1975), 12(6), 1211-13
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Treatment of thioxanthen-9-one 10,10-dioxides I (R = H, Me, MeO) with NaNH2 in liq. NH3 gave dibenzo[b,f][1,4]thiazepin-11(10H)one 5,5-dioxides II (R = H, Me, R1 = H; R = H, R1 = MeO; resp.) II (R = Me, R1 = H) was prepd. from Me 5-methylthiosalicylate.
IT **22871-33-6P 58755-60-5P 58755-62-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and methylation of)
RN 22871-33-6 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5,5-dioxide (6CI, 8CI, 9CI) (CA INDEX NAME)



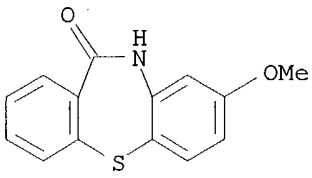
RN 58755-60-5 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



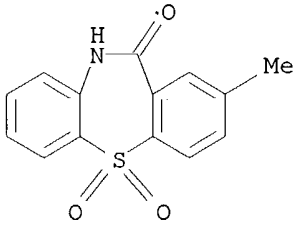
RN 58755-62-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy-, 5,5-dioxide (9CI) (CA INDEX NAME)



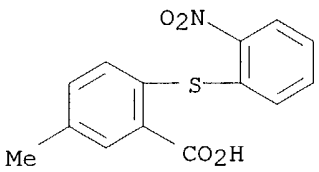
IT **3159-05-5P 58755-60-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)
RN 3159-05-5 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



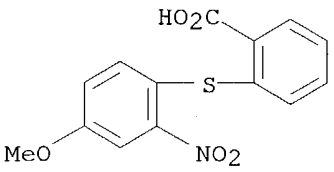
RN 58755-60-5 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



IT **58755-65-0P 58755-67-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
RN 58755-65-0 CAPLUS
CN Benzoic acid, 5-methyl-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)

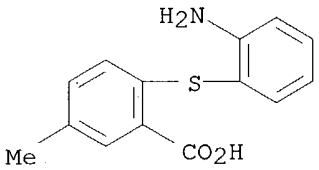


RN 58755-67-2 CAPLUS
CN Benzoic acid, 2-[(4-methoxy-2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)

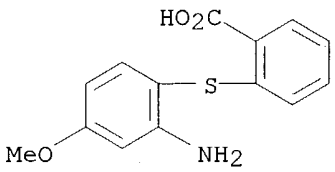


6813

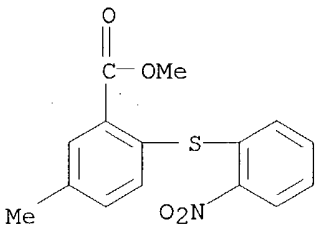
L12 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:105557 CAPLUS
DOCUMENT NUMBER: **84:105557**
TITLE: A novel synthesis of dibenzo[b,f][1,4]thiazepin-11(10H)one 5,5-dioxides
AUTHOR(S): Bennett, O. Francis; Johnson, James; Galletto, Sandra
CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, USA
SOURCE: Journal of Heterocyclic Chemistry (1975), 12(6), 1211-13
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 84:105557
GI For diagram(s), see printed CA Issue.
AB Treatment of thioxanthen-9-one 10,10-dioxides I (R = H, Me, MeO) with NaNH2 in liquid NH3 gave dibenzo[b,f][1,4]thiazepin-11(10H)one 5,5-dioxides II (R = H, Me, R1 = H; R = H, R1 = MeO; resp.) II (R = Me, R1 = H) was prepared from Me 5-methylthiosalicylate.
IT **58755-66-1P 58755-68-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 58755-66-1 CAPLUS
CN Benzoic acid, 2-[(2-aminophenyl)thio]-5-methyl- (9CI) (CA INDEX NAME)



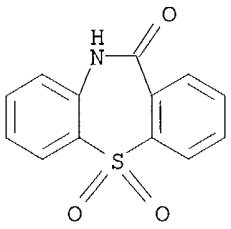
RN 58755-68-3 CAPLUS
CN Benzoic acid, 2-[(2-amino-4-methoxyphenyl)thio]- (9CI) (CA INDEX NAME)



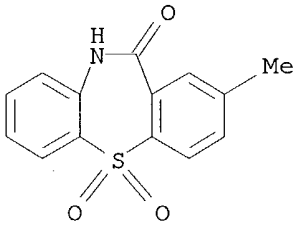
IT **58755-64-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 58755-64-9 CAPLUS
CN Benzoic acid, 5-methyl-2-[(2-nitrophenyl)thio]-, methyl ester (9CI) (CA INDEX NAME)



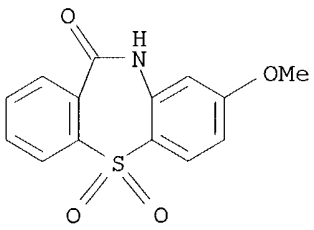
IT **22871-33-6P 58755-60-5P 58755-62-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 22871-33-6 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5,5-dioxide (6CI, 8CI, 9CI) (CA INDEX NAME)



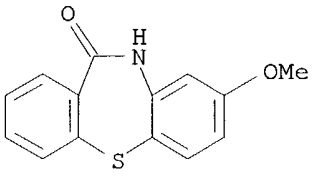
RN 58755-60-5 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



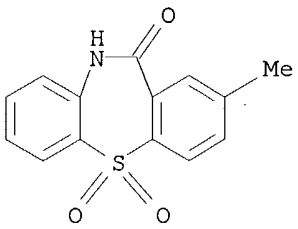
RN 58755-62-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy-, 5,5-dioxide (9CI) (CA INDEX NAME)



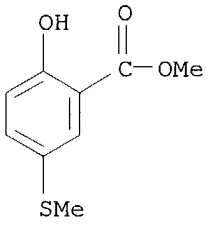
IT **3159-05-5P 58755-60-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
RN 3159-05-5 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



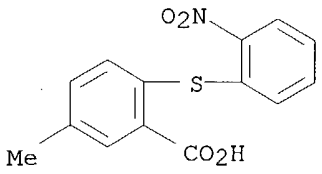
RN 58755-60-5 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



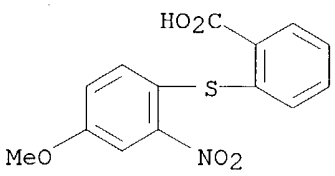
IT **59699-19-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with iodonitrobenzene)
RN 59699-19-3 CAPLUS
CN Benzoic acid, 2-hydroxy-5-(methylthio)-, methyl ester (9CI) (CA INDEX NAME)



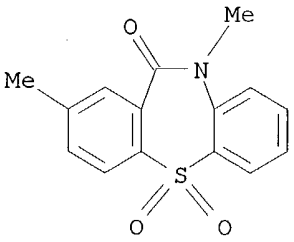
IT **58755-65-0P 58755-67-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 58755-65-0 CAPLUS
CN Benzoic acid, 5-methyl-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



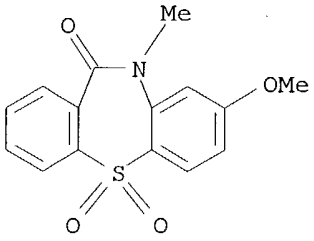
RN 58755-67-2 CAPLUS
CN Benzoic acid, 2-[(4-methoxy-2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



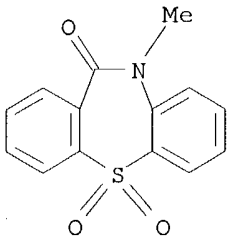
IT **58755-61-6P 58755-63-8P 58790-38-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 58755-61-6 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2,10-dimethyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



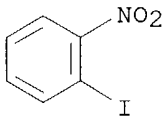
RN 58755-63-8 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy-10-methyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



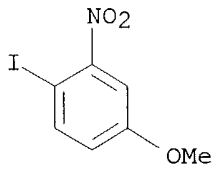
RN 58790-38-8 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 10-methyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



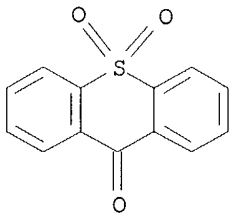
IT **609-73-4 58755-70-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methyl methylthiosalicylate)
RN 609-73-4 CAPLUS
CN Benzene, 1-iodo-2-nitro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



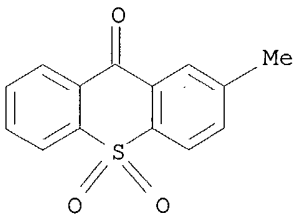
RN 58755-70-7 CAPLUS
CN Benzene, 1-iodo-4-methoxy-2-nitro- (9CI) (CA INDEX NAME)



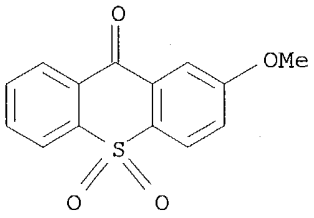
IT **3166-15-2 14753-21-0 58755-69-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sodium amide, dibenzothiazepinone dioxide from)
RN 3166-15-2 CAPLUS
CN 9H-Thioxanthen-9-one, 10,10-dioxide (9CI) (CA INDEX NAME)



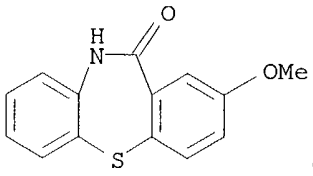
RN 14753-21-0 CAPLUS
CN 9H-Thioxanthen-9-one, 2-methyl-, 10,10-dioxide (9CI) (CA INDEX NAME)



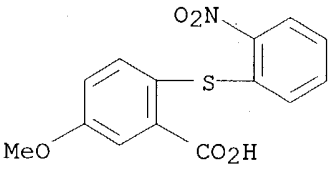
RN 58755-69-4 CAPLUS
CN 9H-Thioxanthen-9-one, 2-methoxy-, 10,10-dioxide (9CI) (CA INDEX NAME)



L13 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1975:140094 CAPLUS
DOCUMENT NUMBER: 82:140094
TITLE: Synthesis of 2-methoxydibenzo[b,f](1,4)-thiazepin-11(10H)-one 5,5-dioxide
AUTHOR(S): Bennett, O. Francis; Johnson, James; Tramondozzi, John
CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, USA
SOURCE: Organic Preparations and Procedures International (1974), 6(6), 287-93
CODEN: OPPIAK; ISSN: 0030-4948
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title compd. (I, n = 2) was prepd. from the nitrobenzoate II (R = Me, R1 = NO2) in 8 steps. Thus II (R = Me, R1 = NO2) was reduced to II (R = Me, R1 = NH2), hydrolyzed to II (R = H, R1 = NH2), deaminated and treated with Na2S to give II (R = H, R1 = SH), which was esterified and treated with 2-O2NC6H4I and hydrolyzed to give II (R = H, R1 = 2.O2NC6H4S). FeSO4-NH4OH redn. gave II (R = H, R1 = 2-H2NC6H4S), which was cyclized to I (n = 0) and oxidized to I (n = 2).
IT **3158-77-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)
RN 3158-77-8 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methoxy- (7CI, 8CI, 9CI) (CA INDEX NAME)

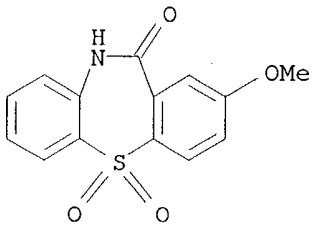


IT **55114-91-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
RN 55114-91-5 CAPLUS
CN Benzoic acid, 5-methoxy-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



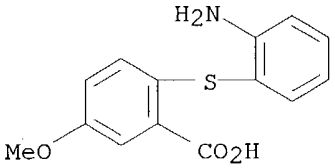
IT **55114-93-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 55114-93-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methoxy-, 5,5-dioxide (9CI) (CA

INDEX NAME)

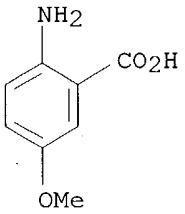


7813

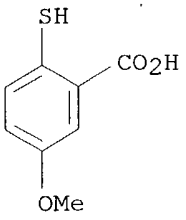
L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:140094 CAPLUS
DOCUMENT NUMBER: **82:140094**
TITLE: Synthesis of 2-methoxydibenzo[b,f](1,4)-thiazepin-11(10H)-one 5,5-dioxide
AUTHOR(S): Bennett, O. Francis; Johnson, James; Tramondozzi, John
CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, USA
SOURCE: Organic Preparations and Procedures International (1974), 6(6), 287-93
CODEN: OPPIAK; ISSN: 0030-4948
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title compound (I, n = 2) was prepared from the nitrobenzoate II (R = Me, R1 = NO2) in 8 steps. Thus II (R = Me, R1 = NO2) was reduced to II (R = Me, R1 = NH2), hydrolyzed to II (R = H, R1 = NH2), deaminated and treated with Na2S to give II (R = H, R1 = SH), which was esterified and treated with 2-O2NC6H4I and hydrolyzed to give II (R = H, R1 = 2.O2NC6H4S). FeSO4-NH4OH reduction gave II (R = H, R1 = 2-H2NC6H4S), which was cyclized to I (n = 0) and oxidized to I (n = 2).
IT **55114-92-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 55114-92-6 CAPLUS
CN Benzoic acid, 2-[(2-aminophenyl)thio]-5-methoxy- (9CI) (CA INDEX NAME)



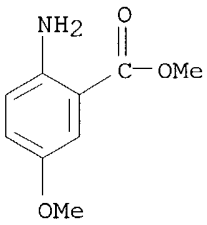
IT **6705-03-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deamination of)
RN 6705-03-9 CAPLUS
CN Benzoic acid, 2-amino-5-methoxy- (9CI) (CA INDEX NAME)



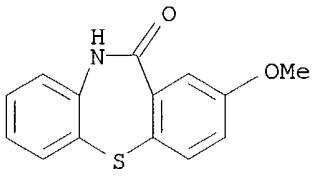
IT **16807-37-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 16807-37-7 CAPLUS
CN Benzoic acid, 2-mercapto-5-methoxy- (9CI) (CA INDEX NAME)



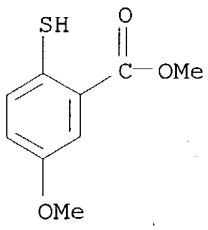
IT **2475-80-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 2475-80-1 CAPLUS
CN Benzoic acid, 2-amino-5-methoxy-, methyl ester (9CI) (CA INDEX NAME)



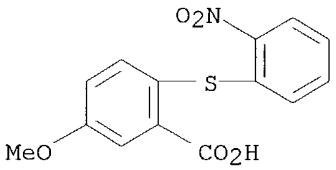
IT **3158-77-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
RN 3158-77-8 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methoxy- (7CI, 8CI, 9CI) (CA INDEX NAME)



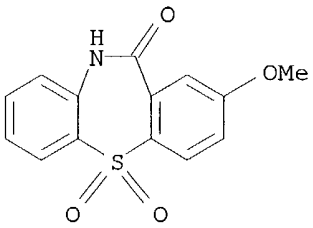
IT **55114-90-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with nitro(iodo)benzene)
RN 55114-90-4 CAPLUS
CN Benzoic acid, 2-mercapto-5-methoxy-, methyl ester (9CI) (CA INDEX NAME)



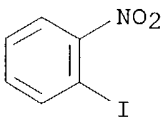
IT **55114-91-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 55114-91-5 CAPLUS
CN Benzoic acid, 5-methoxy-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



IT **55114-93-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 55114-93-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methoxy-, 5,5-dioxide (9CI) (CA INDEX NAME)

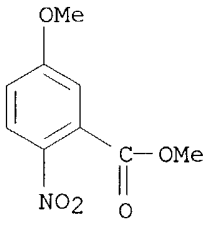


IT **609-73-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methoxythiosalicylate)
RN 609-73-4 CAPLUS
CN Benzene, 1-iodo-2-nitro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **2327-45-9**
RL: RCT (Reactant); RACT (Reactant or reagent)

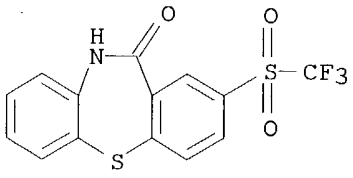
(reduction of)
RN 2327-45-9 CAPLUS
CN Benzoic acid, 5-methoxy-2-nitro-, methyl ester (9CI) (CA INDEX NAME)



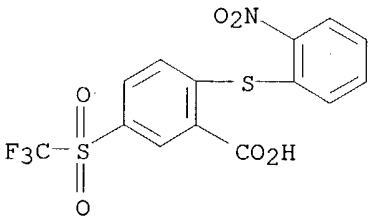
L13 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1974:3563 CAPLUS
DOCUMENT NUMBER: 80:3563
TITLE: Dibenzo[b,f][1,4]thiazepine derivatives
INVENTOR(S): Schmutz, Jean; Hunziker, Fritz; Kuenzle, Franz M.
PATENT ASSIGNEE(S): Wander, Dr. A., A.-G.
SOURCE: Fr. Demande, 27 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2162575	A1	19730720	FR 1972-43707	19721208
FR 2162575	B1	19760702		
CH 560213	A	19750327	CH 1971-17925	19711209
BE 792426	A1	19730607	BE 1972-125052	19721207
JP 48064090	A2	19730905	JP 1972-122128	19721207
GB 1411587	A	19751029	GB 1972-56659	19721208

PRIORITY APPLN. INFO.: CH 1971-17925 19711209
GI For diagram(s), see printed CA Issue.
AB Piperazinyl-benzothiazepines I (R = H, Me, CH2CH2OH, (CH2)3OH, CH2CHMeOH, Et, CH2CH2OMe, CH2CH2OAc) were prepd. for use as sedatives, tranquilizers, antidepressants, and antiemetics. Thus, 2,5-Br(MeS)C6H3CO2H was chlorinated, then fluorinated, and oxidized to 2,5-Br(F3CSO2)C6H3CO2H, which was treated with 2-H2NC6H4SH and cyclized to 2-trifluoromethylsulfonyl-10,11-dihydro-11-oxodibenzo[b,f][1,4]thiazepine. Treatment with 4-methylpiperazine gave I (R = Me).
IT **42252-15-3P 42252-27-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 42252-15-3 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)



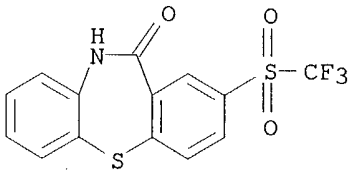
RN 42252-27-7 CAPLUS
CN Benzoic acid, 2-[(2-nitrophenyl)thio]-5-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)


O2N
S
O
F3C
S
O
CO2H

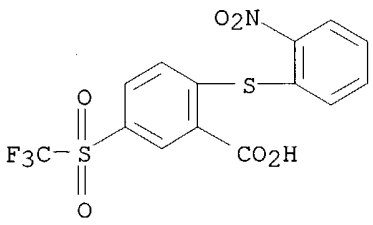
L13 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1973:453389 CAPLUS
DOCUMENT NUMBER: 79:53389
TITLE: 11-Piperazinyl-2-[(trifluoromethyl)sulfonyl] dibenzo[b,f][1,4]-thiazepines
INVENTOR(S): Schmutz, Jean; Hunziker, Fritz; Kuenzle, Franz M.
PATENT ASSIGNEE(S): Wander A.-G.
SOURCE: Ger. Offen., 30 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2259568	A1	19730614	DE 1972-2259568	19721206
CH 560213	A	19750327	CH 1971-17925	19711209
BE 792426	A1	19730607	BE 1972-125052	19721207
JP 48064090	A2	19730905	JP 1972-122128	19721207
GB 1411587	A	19751029	GB 1972-56659	19721208

PRIORITY APPLN. INFO.: CH 1971-17925 19711209
GI For diagram(s), see printed CA Issue.
AB Eight title compds. [I, R = H, Me, Et, CH2CH2OH, (CH2)3OH, CH2CH2OMe, CH2CH2OAc, or CH2CHMeOH] were prepd. by reaction of II or III with piperazines, by cyclization of 2-H2NC6-H4SC6H3(SO2CF3)COA-4,2 (A = piperazinyl residues), and optionally by substitution of I (R = H). I were useful as sedatives, neuroleptics, neurotropic antidepressants, and anti-emetics.
IT **42252-15-3P 42252-27-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 42252-15-3 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)



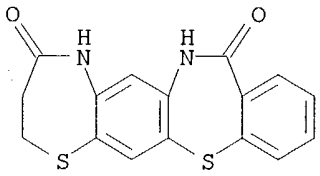
RN 42252-27-7 CAPLUS
CN Benzoic acid, 2-[(2-nitrophenyl)thio]-5-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)



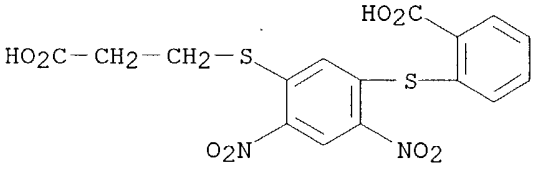
L13 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1966:490113 CAPLUS
DOCUMENT NUMBER: 65:90113
ORIGINAL REFERENCE NO.: 65:16829f-g
TITLE: Nuclear magnetic resonance of benzobisheterocyclic compounds
AUTHOR(S): Grandolini, Giuliano; Ricci, Adolfo; Martani, Alfio; Monache, France Delle
CORPORATE SOURCE: Univ. Perugia, Italy
SOURCE: Journal of Heterocyclic Chemistry (1966), 3(3), 302-10
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The N.M.R. spectra of 49 benzobisheterocyclic compds. containing various heterocycles were detd. The observed spectral data made possible the elucidation of the structure and also clarified the influences of the heterocyclic substituents and of heterocyclic rings on chem. shift values of the aromatic protons. 25 references.

IT **13399-10-5**, 1,5-Benzothiazepino[8,7-b][1,4]benzothiazepine-4,8(5H,7H)-dione, 2,3-dihydro-
(nuclear magnetic resonance of)
RN 13399-10-5 CAPLUS
CN 1,5-Benzothiazepino[8,7-b][1,4]benzothiazepine-4,8(5H,7H)-dione, 2,3-dihydro- (7CI, 8CI) (CA INDEX NAME)



IT **13399-40-1**, Benzoic acid, o-[[5-[(2-carboxyethyl)thio]-2,4-dinitrophenyl]thio]-
(prepn. of)
RN 13399-40-1 CAPLUS
CN Benzoic acid, o-[[5-[(2-carboxyethyl)thio]-2,4-dinitrophenyl]thio]- (7CI, 8CI) (CA INDEX NAME)



L13 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1961:137637 CAPLUS
DOCUMENT NUMBER: 55:137637
ORIGINAL REFERENCE NO.: 55:26001b-i
TITLE: Basically substituted heterocyclic compounds
INVENTOR(S): Hoffmann, Karl; Urech, Ernst
PATENT ASSIGNEE(S): C I B A Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1062246		19590730	DE	
GB 869089			GB	

GI For diagram(s), see printed CA Issue.

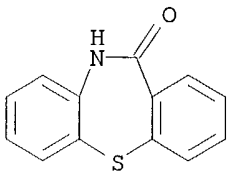
AB 10-(Tertiary-aminoalkyl)-11-oxo-dibenzo[b,f]-1-thia-4-aza-2,6-cycloheptadienes effective as antihistamines and for the treatment of asthma, were made by treating substituted o-nitrochlorobenzenes with an alk. soln. of Me thiosalicylate (I) to prep. Me 2'-nitrodiphenyl sulfide-2'-carboxylate, which gave on redn. the amino analog, which gave by heating the heterocyclic compd., which was treated with reactive aminoalkyl alcs. or esters in the presence of condensing agents, such as alk. metals, their amides or hydrides. Thus, 112 g. I was refluxed in 300 cc. anhyd. MeOH with 17 g. Na 10 min. and then treated with 130 g. 3-nitro-4-chlorotoluene. After refluxing 2.5 hrs., the hot soln. was filtered and cooled to obtain 156 g. Me 2-nitro-4-methyldiphenyl sulfide-2'-carboxylate, m. 140-6.degree.. This compd. (150 g.) gave on hydrogenation in 1100 cc. EtOAc in the presence of 70 g. Ni catalyst 125 g. Me 2-amino-4-methyldiphenyl sulfide-2'-carboxylate, m. 83-5.degree., 60 g. of which was heated at 240-70.degree. for 1 hr., while MeOH was distd. and 40 min. at that temp. in vacuo. After cooling the residue was extd. with 50 cc. anhyd. alc. and filtered to obtain 47 g. II (R2= Me, R = R1 = R3 = H) (III), m. 288-91.degree. (AcOH). A soln. of 28 g. III and 6.4 g. NaNH2 in 300 cc. dioxane was heated 3 hrs. until no more NH3 was formed. After cooling to 60.degree. the stirred mixt. was treated with 22.4 g. .beta.-dimethylaminoethyl chloride in 60 cc. anhyd. benzene within 30 min. and the mixt. refluxed 3 hrs. After filtration of NaCl the filtrate was evapd. in vacuo, the residue dissolved in 200 cc. Et2O, and extd. with dil. HCl. The acid ext. was made alk., the base dissolved in Et2O, dried, and the solvent evapd. to obtain 33 g. II (R2 = Me, R3 = Me2NCH2CH2, R = R1 = H) (IV), m. 109-10.degree. (iso-PrOH-petr. ether), the antihistaminic effect of which was 3 times as great as that of 10-(.beta.-dimethylaminoethyl)phenothiazine in a test on guinea pigs according to the method of Kallos and Pagel. The HCl salt of IV, m. 223-5.degree., was prepd. in EtOAc. The following II were also prepd. (R, R1, R2, R3, % yield, m.p., and m.p. HCl salt given): H, H, Me, iso-PrMeNCH2CH2, 85, 92-3.degree., 209-10.degree.; H, H, Me, Et2NCH2CH290, 72-3.degree., 197-9.degree.; H, H, Me, Me2N(CH2)3, 92, 83-5.degree., 170-2.degree.; H, Me, H, H, -, 272-4.degree., -; H, Me, H, Me2NCH2CH2, 90, 75-6.degree., 236-7.degree.; Me, H, H, H, -, 257-8.degree., -; H, Me, Me, H, -, 303-5.degree., -; H, H, MeO, H, -, 218-19.degree., -; Me, H, H, Me2NCH2CH2, 87, 105-7.degree., 240-1.degree.; H, Me, Me, Me2NCH2CH2, 90, 114-15.degree., 255-7.degree. (decompn.); H, H, MeO, Me2NCH2CH2, -, - (oil), 189-92.degree.; H, H, MeO, Et2NCH2CH2, -, - (oil), 190-2.degree.; H, H, MeO, Me2N(CH2)3, -, 104-6.degree., 141-3.degree.. The following substituted 2'-carbomethoxydiphenyl sulfides were prepd. (substituents and

m.p. given): 2-O2N, 5-Me, 86-8.degree.; 2-H2N, 5-Me, 82-4.degree.; 2-O2N, 6-Me, 100-2.degree.; 2-H2N, 6-Me, 86-7.degree.; 2-O2N, 4,5-Me2, 93-5.degree.; 2-H2N, 4.5-Me2, 130-2.degree.; 2-O2N, 4-MeO, 105-6.degree.; 2-H2N, 4-MeO, 134-5.degree..

IT **3159-07-7**, Dibenzo[b,f][1,4]thiazepin-11(10H)-one (derivs.)

RN 3159-07-7 CAPLUS

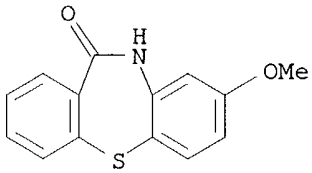
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **3159-05-5**, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy-
29308-82-5, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methyl-
88112-09-8, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 7-methyl-
96953-80-9, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 6-methyl-
97213-14-4, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 7,8-dimethyl-
100726-00-9, Benzoic acid, o-(2-nitro-p-tolylthio)- (prepn. of)

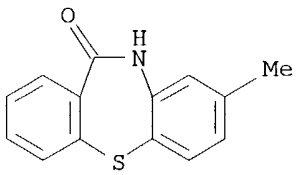
RN 3159-05-5 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



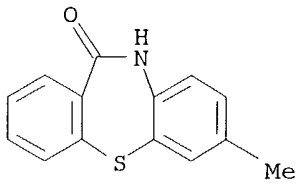
RN 29308-82-5 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methyl- (6CI, 7CI, 8CI) (CA INDEX NAME)

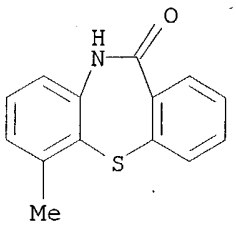


RN 88112-09-8 CAPLUS

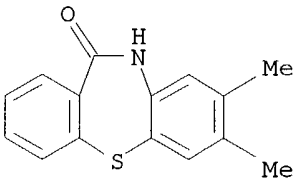
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 7-methyl- (6CI, 9CI) (CA INDEX NAME)



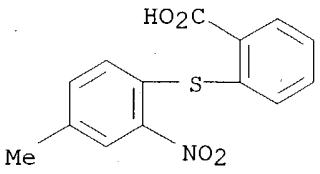
RN 96953-80-9 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 6-methyl- (6CI, 7CI) (CA INDEX NAME)



RN 97213-14-4 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 7,8-dimethyl- (6CI, 7CI) (CA INDEX NAME)

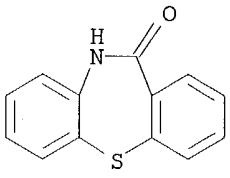


RN 100726-00-9 CAPLUS
CN Benzoic acid, o-(2-nitro-p-tolylthio)- (6CI) (CA INDEX NAME)

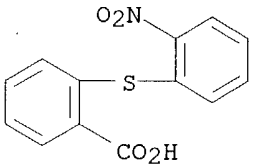


L13 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1958:25574 CAPLUS
DOCUMENT NUMBER: 52:25574
ORIGINAL REFERENCE NO.: 52:4652e-i,4653a-c
TITLE: Antihistamine substances. XLII. Derivatives of 1-aza-4-thia-2,3,5,6-dibenzocycloheptadiene (homophenothiazine)
AUTHOR(S): Hach, Vladimir; Protiva, Miroslav
CORPORATE SOURCE: Pharm. and Biochem. Research Inst., Prague
SOURCE: Chemicke Listy pro Vedu a Prumysl (1957), 51, 1909-14
CODEN: CLPRAN; ISSN: 0366-6832
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 51, 17944a. The authors propose for I (R = H) the name hemophenothiazine and the given numbering system. Adding to MeONa (from 19.0 g. Na and 500 ml. MeOH) 98 g. .omicron.-MeO2CC6H4SH then under stirring and ice-cooling 92.2 g. .omicron.-ClC6H4NO2, heating the mixt. at 50.degree. 15 hrs. under stirring, cooling, combining the sepd. product with the ppt. obtained by dilg. the filtrate with H2O and recrystg. from MeOH gave 94 g. crude Me ester of 2-O2NC6H4SC6H4CO2H-2 (II); pure II m. 92-3.degree.. II (13.8 g.) hydrogenated over PtO2 in 150 ml. 96% EtOH gave the Me ester of 2-H2NC6H4SC6H4CO2H-2 (III), m. 95-6.degree. (75% EtOH). III (20.0 g.) heated in an oil bath 7 hrs. to 200-20.degree. and the solidified molten mass recrystd. (aq. EtOH) gave the lactam (IV) of III, 15.0 g., m. 239-42.degree. (aq. EtOH). Refluxing 30 hrs. a mixt. of 12.0 g. IV, 3.0 g. LiAlH4, and 500 ml. abs. Et2O, cooling, decompg. the mixt. with 35 ml. 10% NaOH, extg. the aq. layer with Et2O, combining the Et2O solns., and evapg. the Et2O gave 10.0 g. I (R = H), m. 115.degree. (EtOH); hydrochloride, m. 175.degree. (EtOH-Et2O). Refluxing 50 ml. of abs. xylene, 7.1 g. I (R = H), 1.9 g. finely ground NaNH2, and 5.5 g. Cl(CH2)2NMe2 10 hrs. in an oil bath, cooling, decompg. the mixt. with 20 ml. H2O, extg. the base with 100 ml. 10% HCl, filtering, extg. the alkalized soln. with C6H6, and evapg. C6H6 gave, on distn., 6.4 g. I [R = (CH2)2NMe2], b0.5 160-5.degree.; hydrochloride, m. 206.degree. (EtOH-Et2O); picrate, m. 156.degree. (EtOH); methiodide, m. 195.degree. (EtOH-Et2O). By an analogous procedure were obtained: N-(2-piperidino-ethyl)homophenothiazine, b0.5 180.degree. [acid succinate, m. 150-1.degree., (EtOH); picrate, m. 165.degree. (EtOH)]; I (R = CH2CH-MeNMe2), b0.5 165-70.degree., 68% [picrate, m. 158.degree. (EtOH)]; I [R = (CH2)3NMe2], b0.5 169-73.degree., 67% [hydrobromide, m. 157.degree.; picrate, m. 135.degree. (EtOH)]. Refluxing 10.5 g. I (R = H), 8.0 g. ClCH2COCl, and 100 ml. C6H6 3 hrs. to 80.degree. gave 11.0 g. I (R = COCH2Cl), m. 103.degree. (EtOH); refluxing the preceding compd. (9.3 g.) with 14 mg. NHEt2 and 120 ml. C6H6 gave 7.8 g. I (R = COCH2NEt2), b0.6 190-5.degree., m. 51-3.degree. (petr. ether); picrate, m. 175.degree. (EtOH); ethobromide, m. 188.degree. (decompn.) (EtOH-Et2O). Refluxing 5.0 g. I [R = CO(CH2)2Cl], m. 98.degree. (EtOH), obtained as above, with 4.0 g. dry MeSNa and 100 ml. abs. Me2CO 6 hrs. on an H2O bath, evapg. the Me2CO, dilg. the residue with H2O, and extg. with C6H6 yielded, on distn., 3.8 g. crude sulfide, b0.8 175-80.degree., which gave, after standing with 15 ml. MeI, I [R = CO(CH2)2S(+)Me2I(-)], m. 133.degree. (decompn.) (EtOH-Et2O). The aminoalkyl derivs. of I are very effective antihistaminics and local anesthetics. The quaternary salts are less effective and practically without local anesthetic effect, but show an antispasmodic activity.
IT **3159-07-7**, Dibenzo[b,f][1,4]thiazepin-11(10H)-one
19806-43-0, Benzoic acid, o-(o-nitrophenylthio)-

(prepn. of)
RN 3159-07-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 19806-43-0 CAPLUS
CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)

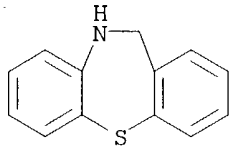


12913

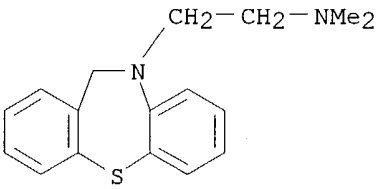
L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1958:25574 CAPLUS
DOCUMENT NUMBER: **52:25574**
ORIGINAL REFERENCE NO.: 52:4652e-i,4653a-c
TITLE: Antihistamine substances. XLII. Derivatives of 1-aza-4-thia-2,3,5,6-dibenzocycloheptadiene (homophenothiazine)
AUTHOR(S): Hach, Vladimir; Protiva, Miroslav
CORPORATE SOURCE: Pharm. and Biochem. Research Inst., Prague
SOURCE: Chemicke Listy pro Vedu a Prumysl (1957), 51, 1909-14
CODEN: CLPRAN; ISSN: 0366-6832
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 51, 17944a. The authors propose for I (R = H) the name hemophenothiazine and the given numbering system. Adding to MeONa (from 19.0 g. Na and 500 ml. MeOH) 98 g. o-MeO2CC6H4SH then under stirring and ice-cooling 92.2 g. o-ClC6H4NO2, heating the mixture at 50° 15 hrs. under stirring, cooling, combining the separated product with the precipitate obtained by diluting the filtrate with H2O and recrystg. from MeOH gave 94 g. crude Me ester of 2-O2NC6H4SC6H4CO2H-2 (II); pure II m. 92-3°. II (13.8 g.) hydrogenated over PtO2 in 150 ml. 96% EtOH gave the Me ester of 2-H2NC6H4SC6H4CO2H-2 (III), m. 95-6° (75% EtOH). III (20.0 g.) heated in an oil bath 7 hrs. to 200-20° and the solidified molten mass recrystd. (aqueous EtOH) gave the lactam (IV) of III, 15.0 g., m. 239-42° (aqueous EtOH). Refluxing 30 hrs. a mixture of 12.0 g. IV, 3.0 g. LiAlH4, and 500 ml. absolute Et2O, cooling, decomposing the mixture with 35 ml. 10% NaOH, extracting the aqueous layer with Et2O, combining the Et2O solns., and evaporating the Et2O gave 10.0 g. I (R = H), m. 115° (EtOH); hydrochloride, m. 175° (EtOH-Et2O). Refluxing 50 ml. of absolute xylene, 7.1 g. I (R = H), 1.9 g. finely ground NaNH2, and 5.5 g. Cl(CH2)2NMe2 10 hrs. in an oil bath, cooling, decomposing the mixture with 20 ml. H2O, extracting the base with 100 ml. 10% HCl, filtering, extracting the alkalized solution with C6H6, and evaporating C6H6 gave, on distillation, 6.4 g. I [R = (CH2)2NMe2], b0.5 160-5°; hydrochloride, m. 206° (EtOH-Et2O); picrate, m. 156° (EtOH); methiodide, m. 195° (EtOH-Et2O). By an analogous procedure were obtained: N-(2-piperidino-ethyl)homophenothiazine, b0.5 180° [acid succinate, m. 150-1°, (EtOH); picrate, m. 165° (EtOH)]; I (R = CH2CH-MeNMe2), b0.5 165-70°, 68% [picrate, m. 158° (EtOH)]; I [R = (CH2)3NMe2], b0.5 169-73°, 67% [hydrobromide, m. 157°; picrate, m. 135° (EtOH)]. Refluxing 10.5 g. I (R = H), 8.0 g. ClCH2COCl, and 100 ml. C6H6 3 hrs. to 80° gave 11.0 g. I (R = COCH2Cl), m. 103° (EtOH); refluxing the preceding compound (9.3 g.) with 14 mg. NHEt2 and 120 ml. C6H6 gave 7.8 g. I (R = COCH2NEt2), b0.6 190-5°, m. 51-3° (petr. ether); picrate, m. 175° (EtOH); ethobromide, m. 188° (decomposition) (EtOH-Et2O). Refluxing 5.0 g. I [R = CO(CH2)2Cl], m. 98° (EtOH), obtained as above, with 4.0 g. dry MeSNa and 100 ml. absolute Me2CO 6 hrs. on an H2O bath, evaporating the Me2CO, diluting the residue with H2O, and extracting with C6H6 yielded, on distillation, 3.8 g. crude sulfide, b0.8 175-80°, which gave, after standing with 15 ml. MeI, I [R = CO(CH2)2S(+)Me2I(-)], m. 133° (decomposition) (EtOH-Et2O). The aminoalkyl derivs. of I are very effective antihistaminics and local anesthetics. The quaternary salts are less effective and practically without local anesthetic effect, but show an antispasmodic activity.

IT **494-20-2**, Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-
6768-40-7, Dibenzo[b,f][1,4]thiazepine, 10-(2-dimethylaminoethyl)-10,11-dihydro- **6768-42-9**, Dibenzo[b,f][1,4]thiazepine, 10-[3-dimethylaminopropyl]-10,11-dihydro- **54920-98-8**, Benzoic acid, o-(o-aminophenylthio)- **112626-08-1**, Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-10-(2-piperidinoethyl)- **113010-99-4**, Dibenzo[b,f][1,4]thiazepine, 10-(N,N-diethylglycyl)-10,11-dihydro-
(and derivs.)

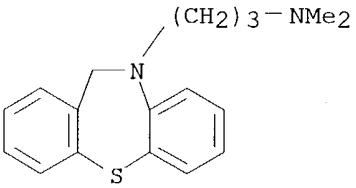
RN 494-20-2 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



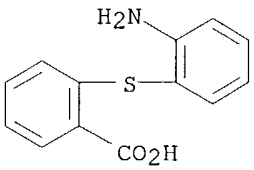
RN 6768-40-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine, 10-[2-(dimethylamino)ethyl]-10,11-dihydro- (6CI, 7CI, 8CI) (CA INDEX NAME)



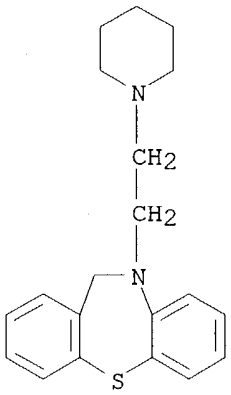
RN 6768-42-9 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine, 10-[3-(dimethylamino)propyl]-10,11-dihydro- (6CI, 7CI, 8CI) (CA INDEX NAME)



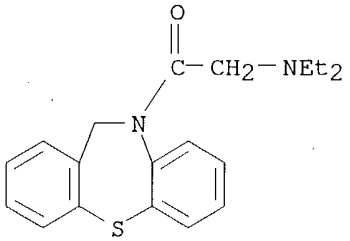
RN 54920-98-8 CAPLUS
CN Benzoic acid, 2-[(2-aminophenyl)thio]- (9CI) (CA INDEX NAME)



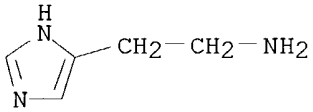
RN 112626-08-1 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-10-(2-piperidinoethyl)- (6CI) (CA INDEX NAME)



RN 113010-99-4 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine, 10-(N,N-diethylglycyl)-10,11-dihydro- (6CI) (CA INDEX NAME)

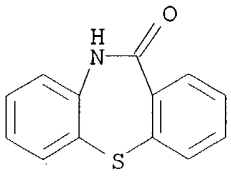


IT **51-45-6**, Histamine
(antihistamine substances)
RN 51-45-6 CAPLUS
CN 1H-Imidazole-4-ethanamine (9CI) (CA INDEX NAME)

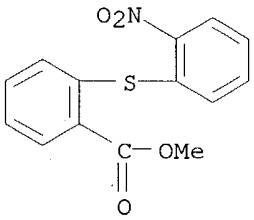


IT **3159-07-7**, Dibenzo[b,f][1,4]thiazepin-11(10H)-one
4892-03-9, Benzoic acid, o-(o-nitrophenylthio)-, methyl ester
19806-43-0, Benzoic acid, o-(o-nitrophenylthio)-
109257-21-8, Dibenzo[b,f][1,4]thiazepine, 10-chloroacetyl-10,11-dihydro- **110178-46-6**, Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-10-[3-(methylthio)propionyl]- **130831-20-8**, Dibenzo[b,f][1,4]thiazepine, 10-(3-chloropropionyl)-10,11-dihydro-
(preparation of)
RN 3159-07-7 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX

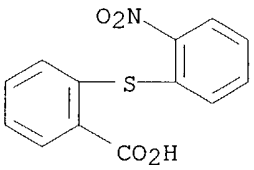
NAME)



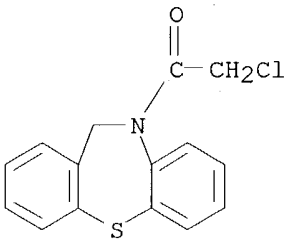
RN 4892-03-9 CAPLUS
CN Benzoic acid, 2-[(2-nitrophenyl)thio]-, methyl ester (9CI) (CA INDEX NAME)



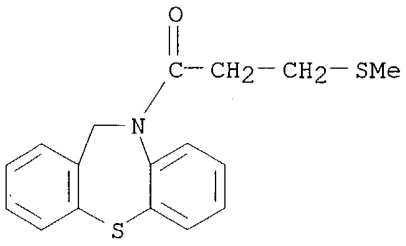
RN 19806-43-0 CAPLUS
CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



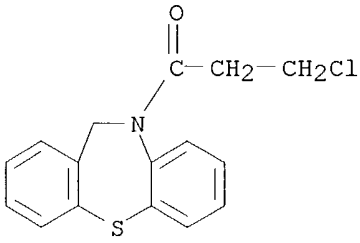
RN 109257-21-8 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine, 10-chloroacetyl-10,11-dihydro- (6CI) (CA INDEX NAME)



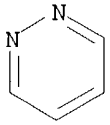
RN 110178-46-6 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-10-[3-(methylthio)propionyl]- (6CI) (CA INDEX NAME)



RN 130831-20-8 CAPLUS
CN Dibenzo[b,f][1,4]thiazepine, 10-(3-chloropropionyl)-10,11-dihydro- (6CI) (CA INDEX NAME)



IT **289-80-5,** Pyridazine
(quaternary derivs.)
RN 289-80-5 CAPLUS
CN Pyridazine (8CI, 9CI) (CA INDEX NAME)



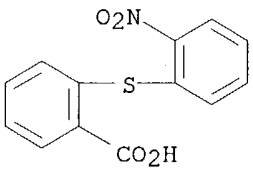
L13 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1958:11111 CAPLUS
DOCUMENT NUMBER: 52:11111
ORIGINAL REFERENCE NO.: 52:2004c-i,2005a-b
TITLE: Beckmann rearrangement of some cyclic sulfone ketoximes
AUTHOR(S): Truce, W. E.; Simms, J. A.
CORPORATE SOURCE: Purdue Univ., Lafayette, IN
SOURCE: Journal of Organic Chemistry (1957), 22, 617-20
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The ease of rearrangement of 10-thiaxanthenone 5,5-dioxide oxime (I), 4-thiachromanone 1,1-dioxide oxime (II), and tetrahydro-4H-1-thiapyran-4-one 1,1-dioxide oxime (III) was found to be III .mchgt. II equal or nearly equal to I. The rearrangement product of I was characterized by independent synthesis. C6H6 and .omicron.-HSC6H4CO2H (IIIa) gave 68% 10-thiaxanthenone (IV), m. 213-14.degree.. IV with H2O2 in AcOH according to Ullmann and von Glenck (C.A. 11, 2668) gave a quant. yield of the 5,5-dioxide (V), m. 187-8.5.degree.. V (10 g.), 16 g. H2NOH.HCl, and 30 ml. C5H5N in 150 ml. alc. refluxed 23 hrs. gave 9.6 g. I, m. 213-14.degree.; shorter reaction times produced a mixt. contg. unreacted V. PCl5 (10.2 g.) in 75 ml. POCl3 refluxed 48 hrs. with 9 g. I in 125 ml. POCl3, the solvent removed, the residue poured into ice H2O, extd. with Et2O, distd., the residue heated 1 hr. with 300 ml. 50% H2SO4, and the product (8.1 g.) heated 1.5 hrs. with 300 ml. 7% NaOH gave 0.9 g. V and 3 fractions: (1) 1.1 g., m. 291-2.5.degree.; (2) 1.5 g., m. 289-91.degree.; (3) 1.7 g., m. 289.5-90.degree.. A mixt. of 1 and 2-(2-H2NC6H4SO2)C6H4CO2H (VI) gave no depression. The yield of VI dropped with a reflux time of 16 hrs., and more V was isolated. A 3-step synthesis, starting with IIIa and .omicron.-O2NC6H4Cl, gave a low yield of VI. IIIa (50 g.) and 15 g. Na in 300 ml. alc. refluxed 4 hrs. with 51 g. .omicron.-O2NC6H4Cl in 300 ml. alc. gave 28.8 g. 2-(2-HO2CC6H4S)C6H4NO2 (VII), m. 166-9.degree.. VII (24 g.) in 200 ml. AcOH treated with 29 ml. 30% H2O2 at such a rate as to maintain gentle reflux, and the mixt. refluxed 3 hrs. and concd. gave 21.5 g. 2-(2-O2NC6H4SO2)C6H4CO2H (VIII), m. 198-200.degree.. VIII (10 g.) suspended in 200 ml. concd. HCl treated under reflux with 23.7 g. Sn, heated 3 hrs. on a steam bath, and the product pptd. by cooling gave 6.7 g. crude VI, m. 287-8.degree. (alc.-AcOH); during drying VI evidently cyclized to the corresponding lactam. Cl(CH2)2CO2H and PhSH gave 83% PhSCH2CH2CO2H (IX). IX gave 68% 4-thiachromanone (X), oxidized with H2O2 in AcOH to 64% of the 1,1-dioxide (XI), m. 128-9.5.degree.. XI (20 g.) similarly treated with H2NOH.HCl in C5H5N and alc. gave 19.1 g. II, m. 193.5-4.5.degree. (from H2O). None of the expected rearrangement product, the lactam (XIa) of 2-H2NC6H4CH2CH2CO2H, was isolated in any of a series of 7 expts. The catalysts, PCl5, 85% H2SO4, 93% H2SO4, and polyphosphoric acid, caused tar formation or hydrolysis to XI. In a no. of cases II was recovered. II was very resistant to hydrolysis or rearrangement when heated with concd. H2SO4. The solvents used for the 7 expts. in order were: POCl3, Et2O, Et2O, CHCl3, 85% H2SO4, 93% H2SO4, and polyphosphoric acid. II (6.33 g.) with 225 ml. H2O and 5.55 g. PhSO2Cl left 19 hrs. at room temp. with 33 ml. N NaOH and refluxed 1 hr. gave 6.05 g. II N-benzenesulfonate (XII), m. 150.5-1.0.degree. (Et2O-CHCl3). XII did not rearrange when heated 0.5 hr. at 140.degree. with polyphosphoric acid; the product contained 20% starting material and tar. XII was recovered quantitatively when heated 6 hrs. at 100.degree. in MeOH in a sealed tube. Concd. HCl 3 hrs. at 120.degree. gave only tar. II (2.10 g.) and 2.33 g. .omicron.-

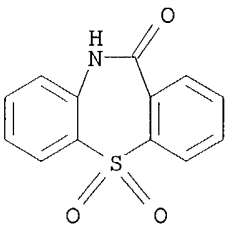
O2NC6H4SO2Cl yielded 3.52 g. of II .omicron.-nitrobenzenesulfonate (XIII), m. 182.5.degree. (decompn.) (dioxane-H2O). XIII (0.90 g.) heated 12 hrs. at 120.degree. with 40 ml. concd. HCl in a sealed tube gave 0.21 g. XIa, m. 243-4.degree. (in alc. pptd. by Et2O). S(CH2CH2CO2Me)2 gave 10% tetrahydro-4H-1-thiapyranone, m. 60-3.degree., oxidized with 30% H2O2 to the 1,1-dioxide (XIV), m. 171.degree.. XIV (3.6 g.), 2.1 g. H2NOH.HCl, and 2.6 g. Na2CO3 in 150 ml. H2O refluxed, then kept 11 hrs., and the solid extd. in a Soxhlet app. gave 1.57 g. III, m. 197-201.degree.. III (1.5 g.) heated 2 min. with 12 ml. 85% H2SO4 gave 1.76 g. MeOH-sol., infusible material, probably H2NCH2CH2SO3K. The mechanism of the above reactions is discussed.

IT **19806-43-0**, Benzoic acid, o-(o-nitrophenylthio)-
22871-33-6, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5,5-dioxide
99847-56-0, Benzoic acid, o-(o-nitrophenylsulfonyl)-
(prepn. of)

RN 19806-43-0 CAPLUS
CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



RN 22871-33-6 CAPLUS
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5,5-dioxide (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 99847-56-0 CAPLUS
CN Benzoic acid, o-(o-nitrophenylsulfonyl)- (6CI) (CA INDEX NAME)